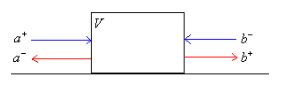
**1D Scattering Matrix**

Consider now possibility of incoming beams on either side – so we would set a+ and b-, and solve for a- and b+. The potential inbetween can be anything, but we will assume the same asymptotic potentials (say 0) on either end. This setup is analogous to the case where we have two beams scattering off of each other, like at the LHC, say. The scattering matrix that we’ll be discussing relates the currents of the incomming beams to those of the outgoing beams. And so we will find it useful to write the wavefunctions on either side in terms of these current (amplitudes).



In terms of the beam density amplitudes, the wavefunctions on either side would be:



but in terms of the current density amplitudes, these would be:



It’s more convenient to write it this way as it makes all the subsequent equations cleaner. The a’s and b’s may be spinors if spin interactions are present. The total current on the left would be:



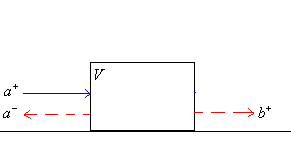
(noting that other stuff is purely imaginary). Similarly, on the other side we’ll get:



So the coefficients of the wavefunction are written so that the a’s, b’s give the currents themselves. Further we can clearly identify the +’s as forward proceeding currents, while the –‘s are backwards proceeding currents. We could observe that if the coefficients am+ and am- are equal/opposite, then we get no net current on that side. And this is sensible b/c then the exponential terms would combine into a standing wave.

**Transmission and reflection matrices**

These coefficients are related via the transmission and reflection matrices, t, r. These are defined via the following experiment. We send a beam of particles towards the sample from the left hand side (defining the a+ coefficients). These either transmit (defining the b+) or reflect back (defining the a- coefficients). And b- = 0 in this experiment.



So these three sets of coefficients are related via:



Alternatively, if we send a beam in from the right then we have:



while a+ = 0 in this experiment. So this t is the transmission matrix in the Landauer formula. Comparing to the earlier current stuff, we see that:



**Current Conservation**

In the first situation, current conservation requires:



The only way this can hold is if the middle is 1 identically. So then we have:



Performing the same analysis on the other side, we would conclude that:



Now let’s consider what should happen under translation. First, the wavefunction will look like this:



Recall the coefficients are related via:

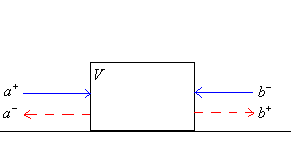


Solving for the new r’s, t’s, etc., we get:



**Scattering matrix**

Both of these situations can be concisely encapsulated in the following matrix relation. Suppose we have sent incoming beams from both sides. The set up looks like this:



Then the outgoing beams would follow from solving the Schrodinger equation. Then it follows that the incoming flux can be related to the outgoing flux via the so-called scattering matrix:



This is consistent with the above two sets of equations. If we let the flux come from the left, then b+ ought to be 0, and the matrix relation reduces to the first set of equations above. And likewise if the flux comes from the right and we set a+ = 0. So these t’s, and r’s are the same as those from above.

**Current Conservation**

The current conservation requirement is the same as the condition of unitarity of the S matrix. Consider:



which brings us to the statement S†S = 1. On the other hand, it must also be true that SS† = 1, because S†S = 1 → SS†SS† = SS† → SS†(SS† - 1) = 0 → SS† = 0, 1. We’ll assume that it isn’t 0. Since both are true we can say that S and S† are inverses of each other. So we can say:



As aside, we can work out the determinant of S…



Anyway, going backwards, we can see that the consequence of this statement is the current conservation law:



which implies that,



The first two identities we’re familiar with. The third is interesting….Writing the statement the other way we have:



This then implies that,



**Time Reversal Symmetry**

Another symmetry we can glean information from is time-reversal symmetry, should it be present. This implies, if ψ(x,t) is a solution then ψ(x,-t)\* is also a solution. Let’s construct the wavefunction.



[bracketed expressions implicitly restricted to left and right of sample] Comparing the coefficients, and noting that the S matrix relation between coefficients holds for all wavefunctions, we see that we should have, for both cases respectively:



We can turn the last equation into the form of the first by multiplying both sides by S† and taking the complex conjugate…



Now compare to the original expression and we see that



The consequence of this is:



and so:



These identities make the above two current conservation equations identical.

**Spin-Rotation Symmetry**

In general the elements of S and M are quaternions, if spin interactions are present, so:



a, b, c, d can be complex - that is, the most general quaternion. Apparently, S (and M?) are self-dual if SRS is present. This would mean that:



(where we have implicitly defined the ‘dual’ operation, and note that a, b, c, d are not required to be real, but if they are, then the quaternion is said to be ‘real’). Therefore self-duality would require that

.

It seems that the dual is a cross between the transpose and the dagger. It transposes, but it doesn’t complex conjugate everything, just the i’s in front of the possibly complex coefficients of the quaternions. The dagger transposes and complex conjugates everything. Of course, the quaternions - **1**, and **σ** - are treated as numbers here, not as matrices, and they don’t get transposed or anything like that. Is it the same for M?

**Parity Symmetry**

What if there were parity symmetry as well? This implies that if ψ(x) is a solution, then ψ(-x) is as well. Note that this doesn’t mean the two wavefunctions are the same. It does mean that the *individual* *eigenfunctions* can be diagonalized by the parity operator, but that they will not all have the *same* parity. So anyway, let’s compare the two wavefunctions.



The scattering matrix describing these two wavefunctions would be:



Again, we can turn the latter into the form of the first via some manipulations:



and so we see that:



which would have the consequence:



which implies:



which would seem obvious in retrospect.

**Summary**

So altogether we have for S:

 (SRS – yes, TRS - yes): S is unitary and symmetric moreover ()

 (SRS – yes, TRS - no): S is unitary

 (SRS – no, TRS - yes): S is unitary and self dual ()

In the β = 1 case, spin is just a spectator – there are no spin terms in H. Additionally, we have TRS, so the transmission coefficient is purely real – only 1 d.o.f. The β = 2 case refers to situations where we might have an L, or p term in H which doesn’t conserve TRS (but not a spin term, presumably). In this case the transmission matrix element can be complex – 2 d.o.f. In the last case, β = 4, we have to explicitly include spin states since we have spin-operators in the Hamiltonian. This gives us 4 d.o.f. in the transmission element since we can have spin up/down for incoming and spin up/down for outgoing.

**Change under translation**

Recalling what we said above,



S would change under translation as follows:



**Polar decomposition of S**

There is a useful way to write S (and M) which separates out the transmission coefficient from the rest. From the unitarity property of S, we can write it in polar form.



U and V are phases, and T = |t|2 is the transmission coefficient. U and V, U′ and V′ have the same symmetries as S in the β = 1, 2, 4 cases. Note how the transmission eigenvalues are degenerate in spin space. This is a consequence of Kramer’s degeneracy. Observe how this form makes sense. On the middle matrix, the left-right diagonal, we just have the reflection eigenvalues (square rooted) which would be r basically. And on the right-left diagonal, we have the square root of the transmission eigenvalues, which is basically t. All we’ve done is separate the transmission/reflection matrices into their magnitudes (middle matrix) and phases (outer matrices). For this reason, its called the polar form – in analogy with the polar representation of a complex number reiφ which separates the complex number into its magnitude times a phase. Now we would like to represent t, t′, r and r′ in terms of this polar decomposition. So we write,



Therefore, we can express the transmission and reflection matrices as



Let’s go the other way and determine the U’s and V’s in terms of the r’s, and t’s, setting U = 1 for convenience. Starting from,



we get:



We see that this polar representation separates information about the wavefunction into two parts. U and V contain information about the input phases of the wavefunction. And U′, V′ contain information about the output phases of the wavefunction (the phase shift basically). Notice how this identification makes sense. r is input (U) times reflection coefficient r ~ √(1-T), times the reflection phase U′. t′ is input from left (U) times transmission coefficient, times output phase to right (V′). And similarly for the others. So altogether we see that S contains information about the phase shifts of the wavefunction in the polar matrices, and about the transmission/reflection coefficients in the ‘radial’ matrix.

**Time Reversal Symmetry**

From the M file, we can see that the consequences of this symmetry are::



And so with TRS we can write **S** as:



and this means that the transmission/reflection coefficients would be given by:



**Caveat for spin interactions**

If spin is important, like with SO interaction (which still preserves TRS because both L and S change sign), then we get the slightly weaker symmetry of ‘self-duality’. Parenthetically, having either/and B and SO involved is called a ‘spin-flip’ process. We have instead of:



rather



where the dual operation is defined as:



**Parity Symmetry**

Check out the M file for details. To summarize, we find that:



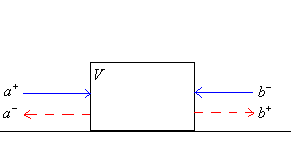
Also that the quantities t + r and t – r are pure phases which we could write as:



and consequently say:



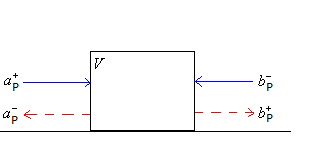
The S-matrix takes a nice form in the parity eigenbasis. To segue, we’ll observe that in our present setup,



we have



and the S-matrix connects the in’s to the out’s. But we’d rather change our basis to parity states so that instead of controlling the incoming left/right waves. We control the incoming +parity/-parity waves, and then see what +parity/-parity outgoing waves we get. So something like (don’t think of the P coefficients as dwelling on just one side of the box – they dwell on both sides simultaneously),



and,



Note the incoming and outgoing basis are both ‘up to us’ to specify. And so we can put the -sgn in front of bP+ if we want to, and we do. The relationship between the two sets of coefficients is:

The bracketed set of equations should be read, ‘amount of a+ we have is amount of aP+ minus amount of bP-‘, etc. So then the Parity basis S-matrix would be:



which we can get from the old one via the manipulations…



(the last ½ is dividing by determinant and all to get the inverse) So



Now in the case where we have Parity symmetry, t´ = t, and r´= r. So this simplifies to a diagonal matrix 😊.



which we can write as,



We’ll find a strong analogy to this in 3D in the angular momentum basis.

**Poles of the phase shift / S-matrix and Levinson’s theorem**

Here’s a few interesting theorems related to the phase shifts and S-matrix.



Apropos analytic continuation, the phase shift usually takes the form of the tan-1(x) function. And it, analytically continued, would be:



I presume the poles of δ± correspond to even/odd energy eigenstates. The bound state energies will necessarily be negative as we can see. The utility of this theorem is that we can experimentally measure the bound state energies of any potential by sending in particles with wavenumbers, k, and measuring the phase shift they acquire. So we can experimentally figure out what δ±(k) is. Then we just apply this theorem and calculate where the poles of δ±(k) are when k is allowed to be a complex number. Given the poles, we just calculate E = ћ2k2/2m for each pole, k, and these are the bound state energies. Also, poles of δ±(k) are also those of the S-matrix of course.



Besides bound states we also frequently encounter metastable, i.e. resonant, states, which are positive energy states with a consequently finite lifetime. An example would be approximate bound states inside two repulsive δ function a distance d apart, say, and with potential strength V. For infinite V, we’d have true bound states, but for finite V, metastable states with a given lifetime. Anyway…



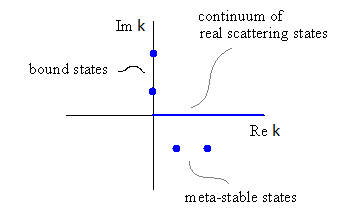
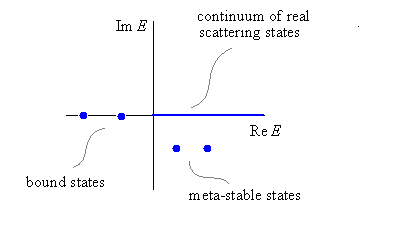
The identification of 1/2τ with -Im() comes from the following. States develop in time according to their energy, exp(-iEt), so if we fill in that complex energy, we get:



from which we recognize the oscillatory phase part as the energy. And when we take the modulus of this factor, we get:



The exponent we’d recognize as the decay rate of the state (presuming Im() < 0). And the lifetime of the state, τ, would be 1/decay rate. Again these would be poles of the S-matrix too. These metastable/resonant states will show up as poles in the lower-half complex plane – otherwise the lifetime would be negative.... a typical plot in the complex k plane, and E plane, is given below.

Consider S as a function of complex k. In the vicinity of a metastable state pole, it will look like this:



The numerator is inferred to be of the indicated form from the fact that S must be a phase (unit magnitude). What does the phase-shift look like in this case?



Now use,



to conclude,



Thus, we can identify metastable states by looking for poles in the argument of the phase shift, with k considered a real variable. The real pole will be the real part of k, and the residue the imaginary part. Then we can construct the energy and lifetime via:

